DEVELOPMENT OF A NMR ^{13}C CHEMICAL SHIFTS PROTOCOL CALCULATION PEFORMING GEOMETRY OPTIMIZATIONS AT THE PM7 LEVEL OF THEORY

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Abstract

Nuclear magnetic resonance (NMR) spectroscopy is one of the most powerful experimental techniques for obtaining three-dimensional structures of complex molecules, mainly for the analysis of the relative and absolute configurations of organic compounds.[1-2] We present a new GIAO-HDFT universal scaling factor and a comparative study in which investigate its ability to predict NMR ^{13}C chemical shifts with low cost-effectiveness ratio. Despite the calculation approximations the chemical shifts calculated at the GIAO-mPW1PW91/3-21G//PM7 using a simple relationship (chemical scalded shifts = 1.14 . chemical shifts calculated – 4.7) were able to yield Mean Absolute Deviation and the Root Mean Square errors as small as those obtained with other GIAO-HDFT with bigger basis sets. The robustness of the new protocol and its applicability to practical problems was evaluated by the calculation of the chemical shifts for two natural compounds with synthesis, biological and therapeutic interest: tryptanthrin and (-)-loliolide. For both compound, the 6 protocols presented good agreement with experimental data. Furthermore, for the second compound, the new protocol performs even better than the 5 others. In conclusion, GIAO-mPW1PW91/3-21G//PM7 linear regression obtained by using the experimental and the calculated data, is a very attractive tool as an alternative to more computationally demanding approaches, which are usually applied in order to achieve ^{13}C NMR chemical shifts calculations.

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2. M. Kaupp (Editor), M. Bühl (Editor), V.C. Malkin (Editor), Calculation of NMR and EPR Parameters. Theory and Applications, Wiley-VCH Verlag GmbH & Co., Weinheim (2004).